

**Summary Statistics for TA\_MH02\_130827:  
Micro-CT Data Acquired at LLNL, Specimen 2 of 3**

Isaac M. Seetho, Kenn E. Morales,  
W. Travis White, III, Harry E. Martz, Jr.  
Lawrence Livermore National Laboratory  
Livermore, CA 94551

Work performed on the  
Science & Technology Directorate of the  
Department of Homeland Security  
Statement of Work  
HSHQPM-10-X-00005 P00007

December 11, 2013  
LLNL-TR-655014



This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

## Executive Summary

TA_MH02_130827				
Measured Density: 1.12 g/cm <sup>3</sup>		X-ray tube voltages (source filter materials)		
Parameter		$\mu_L$ 100 kV(Al), Al-BHC	$\mu_L$ 100 kV(Al), H <sub>2</sub> O-BHC	$\mu_H$ 160 kV (AlCu)
LAC	Mean Measured LAC (LMHU) <sup>1</sup>	1650	1591	1074
	Standard Deviation/Mean	8%	6%	7%
	Entropy	6.36	6.00	5.76
$^L Z_{eff}$	From the mean measured LACs	8.26		
$^{LW} Z_{eff}$	From the mean measured LACs	7.37		
$\mu_L/\mu_H$	Using Al-BHC	1.54		
$\mu_L/\mu_H$	Using H <sub>2</sub> O-BHC	1.48		
QA	From Cu strip and References	Pass		

**Table 1.** First-order statistics of the x-ray linear attenuation coefficient (LAC) in TA\_MH02\_130827, the estimated value of the effective atomic number,  $Z_{eff}$  [1] and  $\mu_L/\mu_H$ .  $Z_{eff}$  is calculated from the ratio of  $\mu_L/\mu_H$ . Beam hardening compensation has been applied to  $\mu_L$  using both aluminum ( $^L Z_{eff}$ ) and water ( $^{LW} Z_{eff}$ ) beam hardening parameters.

Using x-ray micro computed tomography (MicroCT), we have characterized the linear attenuation coefficients (LAC),  $\mu$ , of a sample of a dry powder material, tartaric acid (TA). The specimen was prepared at Lawrence Livermore National Laboratory (LLNL), loaded into a 60mL low density polyethylene (LDPE) bottle. After completed packing, the specimen was scanned following the protocol for MicroCT measurements under Test Plan 79 [2].

This particular specimen, TA\_MH02\_130827, recorded the bulk packing density (mass of sample divided by volume of sample) shown above. Two additional preparations were made and analyzed [3-4]. We used the computer program IMGREC to reconstruct the CT images. The values of the key parameters used in the x-ray data capture and image reconstruction are given in this report. Additional experimental details may be found in the SOP [5] and a separate document [6]. To characterize the statistical distribution of LAC values in each CT image, we first isolated an ~80% region or segment of volume elements (“voxels”) lying completely within the sample, away from the walls of the container. We then calculated the mean value, standard deviation and entropy for (a) the high and low energy image segments and for (b) their digital gradient images<sup>2</sup>. The statistics of the initial image of LAC values are called “first order statistics;” those of the gradient image, “second order statistics.” See Seetho [7] for details of the analysis used to obtain the numbers reported in this document.

<sup>1</sup> LMHU: “LLNL modified Hounsfield units with respect to water.” To obtain the LAC in LMHU for some material at any energy, we multiply by 1000 and divide by the LAC of water at an x-ray energy of 160 kV with aluminum and copper filters.

<sup>2</sup> A digital gradient image of a given image was obtained by taking the absolute value of the difference between the initial image and that same image offset by one voxel horizontally, parallel to the rows of the x-ray detector array.

## Summary of TA\_MH02\_130827 X-ray Statistics

Report Date: December 11, 2013

Report Prepared by: Isaac Seetho  
*Typed or Printed Name*

LLNL  
*Organization*

QA: Isaac Seetho  
*Typed or Printed Name*

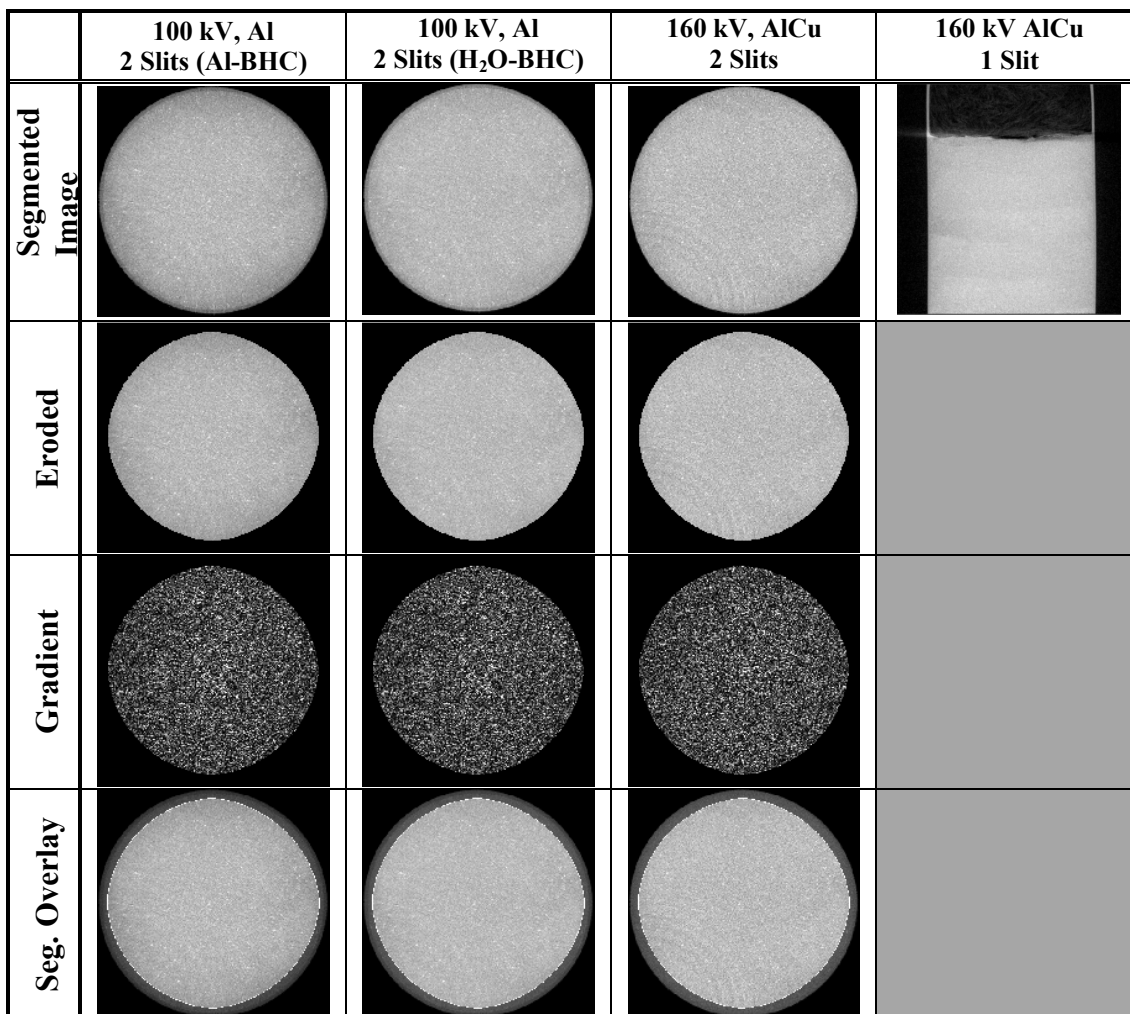
LLNL  
*Organization*

Material ID(s): TA\_MH02\_130827

Source			Collimator	Beam Hardening	Sample Preparation	X-ray Measurement	Linear Attenuation Coefficient (LAC)		
Bias (kV)	Filters		Number of slits	Parameter Source	Date	Date	Statistic	1 <sup>st</sup> order	2 <sup>nd</sup> order
	Material	Thickness							
100	Al	1.943 mm	2	H <sub>2</sub> O	8/9/2013	8/27/2013	Mean Std. Dev. Entropy	1591 98 6.00	76 59 5.31
100	Al	1.943 mm	2	Al	8/9/2013	8/27/2013	Mean Std. Dev. Entropy	1650 140 6.36	89 69 5.47
160	Al Cu	1.943 mm 1.905 mm	2	None	8/9/2013	8/27/2013	Mean Std. Dev. Entropy	1074 77 5.76	65 50 5.15
<sup>L</sup> Z <sub>eff</sub>	Based on measured LAC (Al-BHC)							8.26	
<sup>LW</sup> Z <sub>eff</sub>	Based on measured LAC (H <sub>2</sub> O-BHC)							7.37	
$\mu_L/\mu_H$	Based on measured LAC (Al-BHC)							1.54	
$\mu_L/\mu_H$	Based on measured LAC (H <sub>2</sub> O-BHC)							1.48	

**Table 2.** Key statistics [8] for x-ray measurements of Linear Attenuation Coefficient (LAC). <sup>L</sup>Z<sub>eff</sub> is determined from 100 kV (Al) to 160 kV (AlCu) LAC ( $\mu_L/\mu_H$ ) as given in reference [1]. The statistics here are from the 2-slit image data (not the 1-slit open image data).

Comments: \_\_\_\_\_

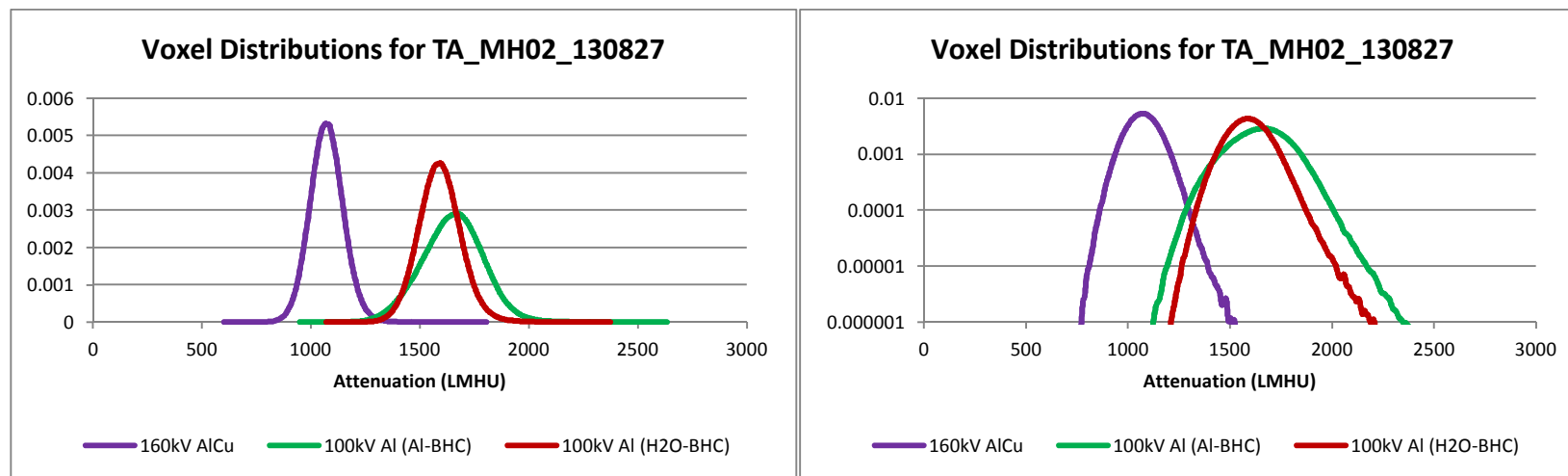


**Figure 1.** X-ray slice images with  $150\mu\text{m} \times 150\mu\text{m} \times 150\mu\text{m}$  voxels. Raw data (top row), segmented images (second row), eroded images (third row) used to calculate first order statistics. Fourth row, difference or gradient image used for second-order statistics. Images not to scale and use different gray scales to obtain maximum contrast. Single slit images (top right) are used for a qualitative visual assessment of homogeneity.

**Comments/Observations on Appearance of Sample (texture, color, other):**

The material has a generally uniform texture. There are visible striations in the vertical full bottle image suggesting nonuniform density values vertically.

## SUPPLEMENTAL ANALYSIS



**Figure 2.** KDE histograms of values of the linear attenuation coefficient (LAC) for TA\_MH02\_130827 for two x-ray source settings (linear plots – left; semi-log plots – right).

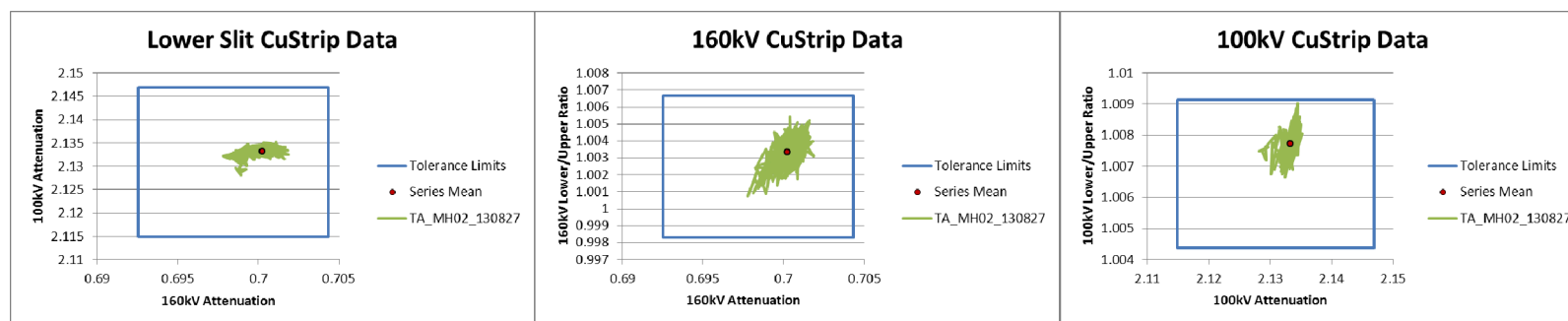
**Comments/Observations on Histograms:** These histograms are made with a Gaussian Kernel Density Estimator (KDE) [8, 9] using 150- $\mu$ m voxel upper-slit CT images.

## Reference Specimens

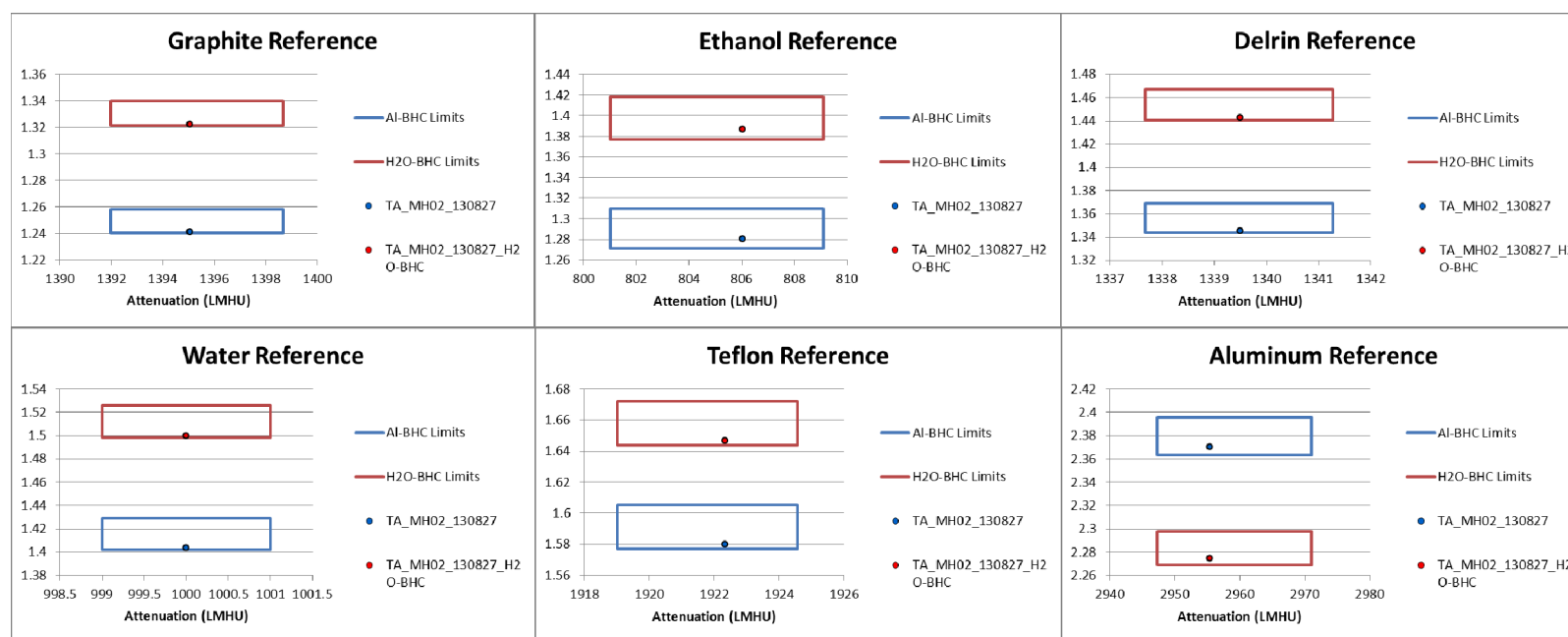
	Parameter	<i>graphite</i>	<i>ethanol</i>	<i>Delrin</i> *	<i>water</i>	<i>Teflon</i> **	<i>aluminum</i> ***
<b>100kV, Al (Al-BHC)</b>	Mean (LMHU)	1732	1032	1802	1404	3037	7005
	Std Dev LMHU)	81	57	82	55	95	139
<b>100kV, Al (H2O-BHC)</b>	Mean (LMHU)	1845	1118	1932	1500	3165	6723
	Std Dev LMHU)	77	58	75	54	69	228
<b>160kV, AlCu</b>	Mean (LMHU)	1395	806	1339	1000	1922	2955
	Std Dev LMHU)	62	48	57	48	60	74

**Table 3.** Linear attenuation coefficients of six reference materials as measured simultaneously with TA\_MH02\_130827.

\* Acetron® GP copolymer. \*\*Enflo Corp. PTFE. \*\*\*T6061 alloy.



**Figure 3.** Copper strip data are within the defined tolerance limits. These tolerance limits were defined using a set of scans spanning from April through May 2013.



**Figure 4.** Reference materials are within the defined tolerance limits. These tolerance limits were defined using a set of scans spanning from April through May 2013.

## Micro-CT System Configuration

1. Scan Location Site: LLNL HEAF
2. Source: Yxlon D09 450 kV Tube; Mfr. Catalog Number: 9421-172-33503; S/N 21-5204
3. Detector: Thales Flashscan 33 with Lanex Fine Gadolinium Oxysulfate Scintillator Screen; s/n 91106194
4. Rotation control system. Controller: Newport Model ESP7000 SN: 1250
5. Carousel: LLNL 2-tray, 6" Dia.
6. Data capture computer: Dell DHM/J4271

## Micro-CT Scan Parameters

1. Scan Geometry:<sup>1</sup> SOD (mm): 1131.0 ODD (mm): 298.7  
Number of positions: 400 Angular Range: 200° Angular Increment: 0.5°
2. Number of Frames averaged per Image: 4
3. Integration time per frame: See p 7.

---

<sup>1</sup> Distances are those recorded in the .sct file for this experiment and are the values used in image reconstruction.



## File Storage Locations for X-ray Data

### Specimen

#### Root Data Path:

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Test\_Data\{sub directory}\

Specimen ID	Date	Radiographer	Slits	kV	mA	Al Filter (mm)	Cu Filter (mm)	Integration <i>dpix</i> Setting [time/frame (s)]	{sub directory}	File Name
TA_MH02_130827	130827	Morales	2	100	1.1	1.943	0	8 [2.8s]	TA_MH02_130827_100Al	TA_MH02_100Al <sub><i>nm</i></sub> .sdt <sup>1</sup>
	130827	Morales	2	160	4.35	1.943	1.905	8 [2.8s]	TA_MH02_130827_160AlCu	TA_MH02_160AlCu <sub><i>nm</i></sub> .sdt
	130827	Morales	1	160	4.35	1.943	1.905	8 [2.8s]	TA_MH02_130827_160AlCu1slit	TA_MH02_160AlCu1slit <sub><i>nm</i></sub> .sdt

### Dark current, mid-range, bright field and $I_o$

#### Root Data Path:

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Test\_Data\{sub directory}\

Slits	kV	Filter	{sub directory}	Dark Image File Name	Mid-Brightness Image File Name	Max Brightness Image File Name	$I_o$ Image File Name
2	100	Al	TA_MH02_130827_100Al	TA_MH02_100Al <sub>drk</sub> R.sdt	TA_MH02_100Al <sub>mid</sub> R.sdt	TA_MH02_100Al <sub>lit</sub> R.sdt	TA_MH02_100Al <sub>bak</sub> .sdt
2	160	AlCu	TA_MH02_130827_160AlCu	TA_MH02_160AlCu <sub>drk</sub> R.sdt	TA_MH02_160AlCu <sub>mid</sub> R.sdt	TA_MH02_160AlCu <sub>lit</sub> R.sdt	TA_MH02_160AlCu <sub>bak</sub> .sdt
1	160	AlCu	TA_MH02_130827_160AlCu1slit	TA_MH02_160AlCu1slit <sub>drk</sub> R.sdt	TA_MH02_160AlCu1slit <sub>mid</sub> R.sdt	TA_MH02_160AlCu1slit <sub>lit</sub> R.sdt	TA_MH02_160AlCu1slit <sub>bak</sub> .sdt

<sup>1</sup> *nm* - is the CT angular index number (0 through 399) for each individual data file

## Reconstruction

**Reconstructed by:** Kenneth E. Morales

**Date:** 8/27/2013

**Location:** LLNL

**Computer:** Dell Precision 690

### Reconstruction Software

**Software:** IMGREC

**Version:** 2.8.1.1c11

**Beam hardening compensation:** Only for 100 kV Al filtered data using Al and H<sub>2</sub>O reference materials for compensation.

### Script Files

LLNL\_script\_TA\_MH02\_100Al.txt

LLNL\_script\_TA\_MH02\_160AlCu.txt

LLNL\_script\_TA\_MH02\_160AlCu1slit\_tw\_WDB.txt

LLNL\_script\_H2OBHC\_TA\_MH02\_100Al.txt

## Reconstructed Specimen Files

### Root Data Path:

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Reconstruction\  
Recon\_130827\{sub directory}\

Slits	kV	Filter	{sub directory}	Reconstruction file name
2	100	Al	TA_MH02_130827_100Al	recobj_ <i>nn</i> <sup>1</sup> .sdt
2	100	Al	H2O_Recon\TA_MH02_130827_100Al	recobj_ <i>nn</i> .sdt
2	160	AlCu	TA_MH02_130827_160AlCu	recobj_ <i>nn</i> .sdt
1	160	AlCu	TA_MH02_130827_160AlCu1slit	recry_ <i>nn</i> .sdt , ry_ <i>nn</i> .sdt

**Observations:** \_\_\_\_\_

<sup>1</sup> *nn* - is the index number for each reconstruction file, modified by an offset corresponding to the frame subsection extracted and analyzed.

## Analysis

**Analysis by:** Isaac Seetho

**Date:** 8/28/2013

**Location:** LLNL

**Computer:** Dell Precision T7500

**Analysis Software**

**Software:** MATLAB

**Version:** R2010b

**GUI Function/Script Files**

micro\_ct\_gui\_1\_3.m<sup>1</sup>

custrip\_gui\_split.m

## Reference & Specimen Analysis Files

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Analyses\  
TA\_MH02\_130827\_analysis\_IMS\_130828\

<b>Analysis File</b>	TA_MH02_130827_characterization.xlsx
----------------------	--------------------------------------

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Analyses\TA\_MH02\_130827\_H2O-  
BHC\_analysis\_IMS\_130828\

<b>Analysis File</b>	TA_MH02_130827_H2O-BHC_characterization_Corrected.xlsx
----------------------	--

## Copper Strip Analysis Files

**Root Data Path:**

\\Working\TP79\_IMXXXXXX\_Microstructure\_Studies\_V1\LLNL\None\HEAFCAT\None\TA\_MH02\_130827\Analyses\  
TA\_MH02\_130827\_custrip\_IMS\_130828\

<b>Aggregate Statistics</b>	Stats_TA_MH02_130827_W80xH7.xls
<b>Mean Value Time Series</b>	Custrip_TA_MH02_130827_W80xH7.xls

<sup>1</sup> Analysis using the MicroCT GUI is done according to the steps outlined in reference [7].

## REFERENCES

1. Jeffrey S. Kallman, Daniel J. Schneberk, Harry E. Martz, Jr., *Two-energy Ratio Method to Determine Zeff from Reference Materials: A Comparison of an Explosive and a Simulant*, Version 3, Lawrence Livermore National Laboratory, LLNL-TR-491153, June 24, 2011.
2. Stephen Azevedo, Jeffrey S. Kallman, Harry E. Martz, Jr., *TP79 – Microstructure Studies Using MicroCT and EDS for DHS R&D*, Lawrence Livermore National Laboratory.
3. Isaac M. Seetho, Kenn E. Morales, W. Travis White, III, Harry E. Martz, Jr., *Summary Statistics for TA\_MH01\_130826: Micro-CT Data Acquired at LLNL, Specimen 1 of 3*, Lawrence Livermore National Laboratory, LLNL-TR-654598, December 11, 2013.
4. Isaac M. Seetho, Kenn E. Morales, W. Travis White, III, Harry E. Martz, Jr., *Summary Statistics for TA\_MH03\_130828: Micro-CT Data Acquired at LLNL, Specimen 3 of 3*, Lawrence Livermore National Laboratory, LLNL-TR-654908, December 11, 2013.
5. “Standard Operating Procedure — Industrial Computed Tomography System Data Collection of Home-Made Explosives,” U.S. Department of Homeland Security Science and Technology Directorate, DHS/STD/TSL-xx-xx, July 9, 2009.
6. Jerel A. Smith, Daniel J. Schneberk, Jeffrey S. Kallman, Harry E. Martz, Jr., David Hoey, *Documentation of the LLNL and Tyndall Micro-Computed-Tomography Systems*, Version 091216, Lawrence Livermore National Laboratory, LLNL-TR-421377, December 17, 2009.
7. Isaac Seetho, *MicroCT: Analysis of CT Reconstructed Data of Home Made Explosive Materials Using the Matlab MicroCT Analysis GUI*, Lawrence Livermore National Laboratory, IDD-MCT-SOP-007, January 13, 2011.
8. Harry E. Martz, Jr., and Carl Crawford, *Validation of Explosive Simulants Requirement Specification*, Version 12, Lawrence Livermore National Laboratory, LLNL-TR-416983-REV 1, October 26, 2009.
9. B. W. Silverman, *Density Estimation*, Chapman and Hall, 1986.